On the spatial density matrix for the centre of mass of a one dimensional perfect gas

B. Carazza

Dipartimento di Fisica dell' Università, viale delle Scienze, I43100 Parma, Italy

INFN Sezione di Cagliari, Italy

Abstract

We examine the reduced density matrix of the centre of mass on position basis considering a one-dimensional system of N non-interacting distinguishable particles in a infinitely deep square potential well. We find a class of pure states of the system for which the off-diagonal elements of the matrix above go to zero as N increases. This property holds too for the state vectors which are factorized in the single particle wave functions. In this last case, if the average energy of each particle is less than a common bound, the diagonal elements are distributed according to the normal law with a mean square deviation which becomes smaller and smaller as N increases towards infinity. Therefore when the state vectors are of the type considered we cannot experience spatial superpositions of the centre of mass and we may conclude that position is a preferred basis for the collective variable.

Key words: Macroscopic states, spatial macrosuperpositions, reduced density matrix, preferred basis, Central Limit Theorem.

1. INTRODUCTION

The old problem of how to derive the classical behaviour of macroscopic bodies from quantum principles now seems much closer to solution thanks to spontaneous localisation theories of the GRW type[1] or by reference to decoherence which occurs for a system interacting with an environment[2].

In the case of a macroscopic body, decoherence is believed to suppress the off-diagonal elements of the spatial reduced matrix of the collective variables, such as the centre of mass, irrespective of initial conditions. This is equivalent to saying that we cannot experience spatial macrosuperpositions of the centre of mass and this explains why we do not encounter states of this kind when looking at everyday objects. Moreover, as long as we limit ourselves to considering spatial distributions of the collective variable and the observable quantities linked to this, we can interpret the reduced density matrix after dechoerence in terms of classical probabilities.

Clearly if pure states exist for a closed macroscopic system, corresponding to a reduced density matrix for the centre of mass that is diagonal on the position basis, they will give the same conclusions for the description of the collective behaviour. This has led us to identify possible pure states of a system of many particles in an external potential with the above graceful property. We wish to make it clear that our purpose is this, not the study of a decoherence process. Decoherence touches us only insofar as the result it gives have provided the inspiration for this note.

For our purposes we require a very simple model as described below. We believe that the final result will be to add something to a genuinely interesting subject, rather than just to present a textbook exercise.

2. A VERY SIMPLE MODEL

The model consists of a closed one-dimensional system of N noninteracting distinguishable particles with position coordinates $x_1, x_2, \cdots, x_N$ in a infinitely deep square potential well $V(x)$. This is actually a one-dimensional ideal gas in a container. The value of $V(x)$ at the bottom of the well is taken as the origin of the energy scale. This region of zero potential occupies the interval $(0, L)$ of the x axis; it is bounded on both sides by infinite potential

barriers.

We will focus our attention on the above case, but will also consider infinitely deep potential wells $U(x)$ represented by an analytical and positive definite function which approach the form of $V(x)$ in some limits. One candidate for $U(x)$ could be:

$$U(x) = [\, 2\,(x - L/2)/L\,]^{2m} \tag{1}$$

with m a positive integer as large as we like it to be.

Apart from the major simplification of no interaction between particles, a further simplification we adopt is to consider the particles as spinless and distinguishable. Each single particle must be identified by its own mass to achieve this, all the masses being different. However, this would introduce a slight but nevertheless unnecessary complication, and we therefore consider particles as having the same mass μ but being of different colours: the visible spectrum does actually offer a large number of possibilities.

Let us consider the energy eigenvalues problem for a single particle in the infinitely deep square potential well. The simple and very known result is the set of eigenfunctions:

$$\varphi_n(x) = \sqrt{2/L}\,\sin(n\pi x/L) \qquad (n = 1, 2, \cdots, \infty) \tag{2}$$

which vanishes at extremes 0 and L and are zero outside the well. These correspond to the discrete energy values:

$$E_n = (n\pi\hbar)^2/(2\mu L^2) \tag{3}$$

and define a vector space for each individual component. A generic state of the system can be expressed using the tensor product space as:

$$\Psi(x_1, x_2, \cdots, x_N) = \sum_{n_1, n_2, \cdots, n_N} c_{n_1, n_2, \cdots, n_N}\, \varphi_{n_1}(x_1)\varphi_{n_2}(x_2)\cdots\varphi_{n_N}(x_N) \quad . \tag{4}$$

Below we consider the factorized state vectors:

$$\Phi(x_1, x_2, \cdots, x_N) = \prod_{i=1}^{N} \psi_i(x_i) \tag{5}$$

with reference to the system subject to the potential $U(x)$ and require that the average energy of each particle is limited by a common bound W:

$$< \psi_i(x_i)|\, \frac{\widehat{p_i^2}}{2\mu} + U(x_i)\,|\psi_i(x_i) >= \frac{<\widehat{p_i^2}>}{2\mu} + < U(x_i) > \leq W \tag{6}$$

where $\widehat{p}_i$ is the momentum operator of the i^{th} particle. Since the average potential energy is positive, it follows that $< \widehat{p_i^2} > \leq 2\mu W$ and clearly the mean square deviation of the momentum $< \widehat{p_i^2} > - < \widehat{p}_i >^2 \leq 2\mu W$. Now indicating with $\sigma_i =< x_i^2 > - < x_i >^2$ the mean square deviation for the position of the i^{th} particle the uncertainty relation imply that $\sigma_i \geq \hbar^2/(8\mu W)$ for each i. This will be valid still in the limiting case of infinitely deep square well.

3. THE REDUCED MATRIX FOR THE CENTRE OF MASS

As we are interested in the collective behaviour of the system, we will use the position co-ordinate of the centre of mass:

$$X = (x_1 + x_2 + \cdots + x_N)/N$$

and the coordinates ξ_i of the particles with respect to their centre of mass: $x_i = X + \xi_i$. The ξ_i are not independent, since they must satisfy the relation $\sum_{i=1}^{N} \xi_i = 0$. We will consider as independent variables X together with the first $N-1$ relative co-ordinates, i.e. $\xi_1, \xi_2, \cdots, \xi_{N-1}$. The last relative co-ordinate is expressed as $\xi_N = -\sum_{i=1}^{N-1} \xi_i$. The Jacobian determinant of the transformation is equal to N. We will write the integration volume element for the new variables as $dV = dV_c\, dV_b$, where $dV_c = dX$ refers to the centre of mass and $dV_b = N d\xi_1\, d\xi_2 \cdots d\xi_{N-1}$ to the internal degrees of freedom. The trace operations in which the continuous spatial reduced matrix of the centre of mass may be involved will therefore be executed using the integration element dX.

We now consider a state vector of the system, $\Psi(x_1, x_2, \cdots, x_N)$. Its projection $< X'|\Psi >$ on a position eigenstate $|X' >$ of the centre of mass is simply $\Psi(X + \xi_1, X + \xi_2, \cdots, X + \xi_{N-1}, X - \sum_{i=1}^{N-1} \xi_i)$. The reduced density matrix elements we are interested in are obtained by taking the partial trace of $< X'|\Psi >< \Psi|X >$ over the microscopic degrees of freedom:

$$\varrho_{X'X} = \int \Psi^*(X + \xi_1, \cdots, X - \sum_{i=1}^{N-1} \xi_i)\Psi(X' + \xi_1, \cdots, X' - \sum_{i=1}^{N-1} \xi_i)\, dV_b \quad (7)$$

or taking the relation $\sum_{i=1}^{N} \xi_i = 0$ into account with the aid of a delta function:

$$\varrho_{X'X} = N \int \delta(\sum_{i=1}^{N} \xi_i) \Psi^*(X+\xi_1, \cdots, X+\xi_N) \Psi(X'+\xi_1, \cdots, X'+\xi_N)\, d\xi_1 \cdots d\xi_N \tag{8}$$

4. THE OFF DIAGONAL ELEMENTS

We will now look at the off diagonal elements $\varrho_{X'X}$. In the first place, we note that these are limited to the range $(0, L)$ of X and X'. This is clear from observing Eq. (8) and remembering that the wavefunctions of the system are zero when the position coordinates x_1, x_2, $\cdots, x_N$ are outside this range. We may also note that, for the same reason, only the integration region for which both inequalities $-X < \xi_i < L - X$ and $-X' < \xi_i < L - X'$ are satisfied for each i may contribute to the integral in Eq. (8) which defines the matrix elements. Let $X' > X$ and $\Delta = X' - X$. Therefore, indicating as Ω the volume spanned by the values of the ξ_i in the intervals $-X \leq \xi_i \leq L - X'$ and using the expression in Eq. (4) for the generic state vector:

$$\varrho_{X'X} = N \sum_{n_1,\cdots,n_N} \sum_{m_1,\cdots,m_N} c^*_{n_1,\cdots,n_N}\, c_{m_1,\cdots,m_N}\, I_{n_1,\cdots,n_N;m_1\cdots,m_N} \tag{9}$$

where

$$I_{n_1,\cdots,n_N;m_1,\cdots,m_N} = \int \delta(\sum_{i=1}^{N} \xi_i) \prod_{i=1}^{N} \varphi^*_{n_i}(X+\xi_i) \prod_{j=1}^{N} \varphi_{m_j}(X'+\xi_j)\, d\Omega \quad . \tag{10}$$

Applying the Schwartz inequality:

$$|I_{n_1,\cdots,n_N;m_1,\cdots,m_N}|^2 \leq \int \delta(\sum_{i=1}^{N} \xi_i) \prod_{i=1}^{N} |\varphi_{n_i}(X+\xi_i)|^2\, d\Omega \int \prod_{j=1}^{N} |\varphi_{m_j}(X'+\xi_j)|^2\, d\Omega \tag{11}$$

Since the term to be integrated in the first factor is a definite positive quantity, we can remove the delta function which restricts the integration region and obtain a fortiori:

$$|I_{n_1,\cdots,n_N;m_1,\cdots,m_N}|^2 \leq \prod_{i=1}^{N} \int_{-X}^{L-X'} |\varphi_{n_i}(X+\xi_i)|^2\, d\xi_i \prod_{j=1}^{N} \int_{-X}^{L-X'} |\varphi_{m_j}(X'+\xi_j)|^2\, d\xi_j \tag{12}$$

If the integration variables are changed the previous expression may be rewritten as:

$$|I_{n_1,\cdots,n_N;m_1,\cdots,m_N}|^2 \leq \prod_{i=1}^{N} \int_0^{L-\Delta} |\varphi_{n_i}(x_i)|^2 \, dx_i \prod_{j=1}^{N} \int_{\Delta}^{L} |\varphi_{m_j}(x_j)|^2 \, dx_j \quad . \quad (13)$$

Now if we use δ_Δ to indicate the maximum value with respect to the index n of the quantity:

$$\int_0^{L-\Delta} |\varphi_n(x)|^2 \, dx = \int_{\Delta}^{L} |\varphi_n(x)|^2 \, dx = 1 - \int_0^{\Delta} |\varphi_n(x)|^2 \, dx$$

where we used the simmetry properties of the $\varphi_n(x)$ and the fact that the same wavefunctions are normalized, we finally have:

$$|I_{n_1,\cdots,n_N;m_1,\cdots,m_N}| \leq \delta_\Delta^N \quad . \quad (14)$$

To return to the Eq. (9) above and using the triangular inequality we finally obtain:

$$|\varrho_{XX'}| \leq N \, S \, \delta_\Delta^N \quad (15)$$

where S indicates the double sum:

$$\sum_{n_1,\cdots,n_N} \sum_{m_1,\cdots,m_N} |c_{n_1,\cdots,n_N}| \, |c_{m_1,\cdots,m_N}| = (\sum_{n_1,\cdots,n_N} |c_{n_1,\cdots,n_N}|)^2 \quad .$$

Quantity δ_Δ is clearly less than one for each finite value of Δ. Therefore, if the value of S is given by a polynomial in N, the non-diagonal matrix elements tend to zero in the limit of large N. The results obtained refer to those matrix elements for which $X' \geq X$, but may also be extended immediately to the other half, remembering that our matrix is hermitean.

If only a number l of terms appear in the expression of the generic state vector, one can easily see that, given the normalisation constraint, the maximum possible value for S is l. Therefore, the condition required to have a corresponding spatial reduced density matrix for the centre of mass which is diagonal is clearly satisfied by the fundamental state, by the low-lying energy eigenstates and by their superpositions.

In the case of a factorized state vector as in Eq. (5), by applying the Schwartz inequality once again and after some calculations like above, we

obtain:

$$|\varrho_{X'X}|^2 \leq N^2 \prod_{i=1}^{N} \left(1 - \int_{L-\Delta}^{L} |\psi_i(x_i)|^2 \, dx_i\right) \prod_{j=1}^{N} \left(1 - \int_{0}^{\Delta} |\psi_j(x_j)|^2 \, dx_j\right) \quad . \tag{16}$$

If we exclude very unusual forms of the $\psi_i(\xi_i)$ functions, all factors on the right-hand side are less than unity and their product therefore decreases rapidly as N increases. To be more precise, we assume that the particles have the same individual wave function. In which case:

$$|\varrho_{X'X}| \leq N a_{\Delta}^{N/2} b_{\Delta}^{N/2} \tag{17}$$

with a_Δ, b_Δ positive quantities less than one for any finite Δ and the off-diagonal matrix elements exponentially tending to zero as N increases.

5. THE DIAGONAL ELEMENTS FOR FACTORIZED STATES

We will now examine the diagonal elements of the reduced matrix, with the reference only to a factorized state vector as indicated in Eq. (4), as this is the only case in which we can obtain specific results. Using Eq. (8) and the Fourier representation of the delta function, we have:

$$\varrho_{XX} = \frac{N}{2\pi} \int dk \prod_{i=1}^{N} \int e^{ik\xi_i} \psi_i^*(X + \xi_i) \psi_i(X + \xi_i) \, d\xi_i \tag{18}$$

which may be rewritten as:

$$\varrho_{XX} = \frac{N}{2\pi} \int dk e^{-ikNX} \prod_{i=1}^{N} \int e^{ikx_i} \psi_i^*(x_i) \psi_i(x_i) \, dx_i \quad . \tag{19}$$

Apart from the factor N (since we are using the differential element dX instead of dY here), this is nothing other than the expression for the probability density distribution of the sum $NX = Y = x_1 + x_2 + ... + x_N$. We could have written this directly using the characteristic functions method by observing that the x_i are distributed in accordance with the N independent probability densities $F_i(x_i) = \psi_i^*(x_i)\psi_i(x_i)$.

We will now consider the second central moments $\sigma_i = < (x_i - < x_i >)^2 >$ and the sum $s_N = \sum_{i=1}^{N} \sigma_i$. If we require that the average energy $< E_i > \leq W$

for each particle, it follows as noted that the second central moments are limited by a common bound independent of N. This means $\sigma_i \geq \alpha$ were α is a positive constant.

In the case of the infinitely deep square well, since the $F_i(x_i)$ are carried by a finite interval, the only requirement that each $\sigma_i \geq \alpha$ is sufficient to satisfy the Lindeberg condition[3] for the Central Limit Theorem (CLT). Therefore, under the conditions indicated, the distribution of the diagonal elements ϱ_{XX} will be well expressed for a very large N by the Gaussian:

$$\sqrt{\frac{N}{2\pi < \sigma >}}\, e^{-N(X-<X>)^2/2<\sigma>} \tag{20}$$

where $< \sigma >$ indicates the quantity s_N/N and $< X >= \sum_{i=1}^{N} < x_i > /N$ is the average value of the centre of mass position. $< X >$ and $< \sigma >$ will depend generally on time, but the Gaussian form for large N will in any case be guaranteed since the conditions for the CLT are satisfied independently of time. Moreover, as the wave functions are zero outside the interval $(0, L)$, the particles mean square deviations are also limited from above. We certainly have $\sigma_i \leq L^2$ for each particle. Therefore $< \sigma >= \sum_{i=1}^{N} \sigma_i/N$ remains limited and $< \sigma > /N$ goes to zero as N increase. On the time dependence of the central value $< X >$ and of the variance it can be said that this dependence will be of the periodic type, since the Bohr frequencies involved are whole multiples of a basic frequency, as can be seen from Eq. (3)

In the case of the potential $U(x)$, we once again find that the distribution of diagonal matrix elements follows the normal law if in addition to the requirement that the average energy of each particle is limited (which means that their second central moments are limited as well) we also consider the third absolute central moments $\nu_i =< \mid x_i - < x_i > \mid^3 >$ and make the physically reasonable assumption[4] that $\nu_i \leq \beta$ for some positive constant β. Indeed in this case the Liapunov conditions for the CLM[5] are satisfied.

6. FINAL REMARKS

We have considered the reduced density matrix of the centre of mass on position basis corresponding to the pure states of a one-dimensional system of non-interacting distinguishable particles in an infinitely deep square well

potential. By expressing the generic state vector in terms of energy eigenstates, a sufficient condition was identified for the matrix in question to be diagonal. The condition is that the quantity S defined in the text is limited by a polynomial in the number N of particles. This is clearly satisfied by the fundamental state, by the low-lying energy eigenstates and by their superpositions. Therefore, when the system is in one of these pure states, or others for which the condition on S is verified, we cannot experience spatial superpositions of the centre of mass, its spatial reduced density matrix can be thought of in terms of classical probability and to conclude the position will appear as a preferred basis for the collective variable. However we are cautious about this last conclusion, since non-diagonal elements of "small" subsystems are known to be small in an arbitrarily chosen basis. There even exist theorems for the most probable value of entropy of such systems[6].

Since we expressed the generic state vector by means of energy eigenstates the coefficients of the expansion depend on time only by way of a phase factor, and as S depends on their moduli when the condition required for this quantity is satisfied, it is satisfied permanently. The above states for our system of non-interacting particles do not therefore appear to be the final result of a decoherence process. Nevertheless, if we introduce an interaction between the particles (implying a time dependence for the moduli of our expansion coefficients) we could think of the possible states which evolve fulfilling at the end the condition on S as the result of a process of decoherence, considering our gas as consisting formally of a "collective system" described by the centre of mass and an (internal) environment described by the microscopic degrees of freedom. Coupling between the two formal systems is guaranteed by the external potential.

We also considered the case in which the system's state vector is factorized in the individual wave functions of its components. This state vector is a long way from being generic, but this assumption is natural if there is no interparticle interaction. Here too there are indications that the corresponding spatial reduced density matrix of the centre of mass is diagonal. Moreover, if we require the average energy of each particle to be less than a common value, the conditions for the CLT are satisfied and the diagonal elements of the matrix considered are well expressed by a Gaussian distribution as N increase. The Gaussian parameters are time dependent, but the mean square deviation decreases in any case as $1/N$. This is consistent with a recent work in which we discussed the localisation properties of a

macroscopic body with low total average energy[7]. Factorised states of such a type appear for any practical purpose as localised states of the centre of mass. Each of them appears potentially to be the result of successive spontaneous random localisations of the individual particles, as contemplated by theories of the GRW type. An appropriate classical probability distribution of similar states localised at various values of the position can at a given moment mimic the distribution of diagonal elements of the reduced matrix corresponding to the states considered before. But the meaning of the two cases is very different[8].

To conclude, we must remember that some time ago, the example of a macroscopic ball bouncing elastically between two parallel walls positioned normally to the x axis was used to demonstrate the difficulties encountered in describing a similar situation with quantum mechanics[9]. The gas in our example cannot be considered a compact body like a ball, but we agree that it is macroscopic. If this is described by a factorised state vector like those indicated the centre of mass position is distributed according to a well localised Gaussian, whose central value moves with periodic motion between the two walls. However we do not claim that this distribution, which is a general consequence of the statistical independence of the particles, represents classical behaviour which would require a Gaussian distribution about a time-dependent centre for each wave function in the ensemble. This could be expected only for a bound state describing a macroscopic object, not for a gas.

References

[1] G.C. Ghirardi, A. Rimini, T. Weber *Phys. Rev.* **D 34**, 470, (1986); P. Pearl, *Phys. Rev.* **A 39**, 2277 (1989); G. C. Ghirardi, P. Pearle, A. Rimini *Phys. Rev.* **A 42**, 78 (1990)

[2] W. H. Zurek, *Phys. Rev.* **D 26** (1982) 1862; E. Joos and H. D. Zeh, *Zeits. Phys.* **B 59** (1985) 223; A. O. Caldeira and A. J. Legget, *Phys. Rev.* **A 31** (1985) 1059; W. H. Zurek, *Physics Today* **44** (1991) 36, *ibid*,**46** (1993) 81; W. H. Zurek, *Prog. Theor. Phys.* **89** (1993) 281; J. P. Paz and W.

H. Zurek, *Phys. Rev.* **D 48** (1993) 2728; R. Omnes, *The Interpretation of Quantum Mechanics* Princeton Un. Press (1994), chap. 7.

[3] W. Feller, *An Introduction to Probability Theory and Its Applications* (John Wiley & Sons 1966) p. 264.

[4] M. Tegmark and H. S. Shapiro, *Phys. Rev.* **E 50** (1994) 2538.

[5] A. Reny, *Foundations of Probability* (Holden-Day, San Francisco 1970).

[6] Don N. Page, *Physical Review Letters* **71** (1993) 1291.

[7] B. Carazza *Foundations of Physics Letters* **9** (1996) 79.

[8] B. d'Espagnat *Foundations of Physics* **20** (1990) 1147.

[9] M. Jammer, *The Philosophy of quantum Mechanics* (John Wiley & Sons, New York 1974) p. 218